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Dynamic convexity for natural thermostatted systems

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Dedicated to the memory of José Luis Massera (June 8, 1915–September 9, 2002)

Abstract

Natural thermostatted systems are mechanical systems whose Lagrangian is the difference of a kinetic and a potential energy, subjected to the nonholonomic constraint of a constant kinetic energy. When any two points of the configuration space are joined by a thermostatted motion, we say that the system is *dynamically convex*. A thermostatted charged particle on the plane with a constant electric field is not a dynamically convex system. We prove a general *sufficient condition* for dynamic convexity, from which whole classes of examples are easily constructed.

Keywords: Nonholonomic dynamics; Thermostats; Hopf–Rinow theorem

1. Introduction

Lagrangian systems with constraints on the velocities, called *nonholonomic*, are more and more studied both for the theory and the applications, see [2,6,8,9], and the references therein.

The lack of a true variational principle for nonholonomic systems is so unpleasant that a new model was introduced: vakonomic mechanics. However, inspite of the rich mathematics, there do not seem to exist examples for that theory in the strict framework of analytical mechanics of constrained systems, as discussed in [13].

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So, I guess we should accept the fact that some physical theories may fail to be variational, like nonholonomic constrained mechanics. This conclusion holds for the general theory, even for constraints linear in the velocities. However, some nonholonomic constraints may have variational character. A noteworthy class is given by the *Gaussian isokinetic thermostat* as proved by Dettmann and Morriss [4].

The present paper considers natural Lagrangian functions, namely the difference between a general kinetic energy (quadratic in the velocities) and a potential one. We first write equations, without Lagrangian multipliers, for the systems defined by natural Lagrangian functions and by the nonholonomic constraint of a constant kinetic energy, so called *natural thermostatted systems*. This is done in a way already shown in [13] for general nonlinear nonholonomic constraints, and used in the clear [3] to study the instability of equilibria. Then we extend to natural thermostatted systems the geodesic dynamics found by Dettmann and Morriss [4] in the noteworthy case of Euclidean kinetic energy.

Our main aim is to study the *dynamic convexity* of the thermostatted systems. We say that a thermostatted system is dynamically convex if, for any given pair of points in the configuration space, there exists a thermostatted motion which joins them. This is not true for a thermostatted charged particle on the plane with a constant electric field which is part of the known model of electric conduction called *Lorentz gas* (see [4]). We revisit this example using a complex variable technique which gives the thermostatted motions in a straightforward way.

If we remove from that system the potential energy, and also the nonholonomic constraint (which plays no role without potential energy), we get a free particle which is dynamically convex unlike the thermostatted particle above. Of course, both dynamics keep a constant value of the kinetic energy.

The contrary situation may also happen: Example 3.2 shows a thermostatted system which is dynamically convex while the unconstrained dynamical system with the same kinetic energy and no potential is not.

We give three sufficient conditions for dynamic convexity. The first one, Proposition 3.1, introduces some of the ideas. As a consequence we can deal with Example 3.2.

The second statement, Theorem 3.3, is the bulk of the paper and gives a sufficient condition of dynamic convexity on open connected subsets of $\mathbb{R}^n$, by means of certain auxiliary functions. As a corollary we can get also the previous simpler Proposition 3.1 which we prefer to anticipate to introduce the ideas gently. Theorem 3.3 seems a general tool to deal with dynamic convexity of thermostatted systems. For instance, we get the example, in formula (3.16), with trivial kinetic energy and with the potential energy $U(x) = \frac{1}{2}\log(1 + |x|^2) + f(x)$, $x \in \mathbb{R}^n$, where f is an arbitrary bounded from above smooth function. These functions give dynamically convex thermostatted systems.

Section 4 shows that all the content of the paper finds its most general setting on Riemannian manifolds. We consider the equations for the dynamics of thermostatted systems in this general framework and state and prove our most general result: Theorem 4.1. The proof needs only small modifications and few easy arguments added to the previous demonstration of Theorem 3.3, nothing essentially new. Of course the results of Section 4 are more general and satisfactory than the ones in the previous section. We refrained from writing all the paper within Riemannian geometry in order to try to keep the attention of the reader not acquainted with differential geometry. That is why we also provided a new (simpler than the original) proof for Gordon's result [5] which is inserted in the proof of Theorem 3.3 to have a self-contained paper.

Finally, let us mention that thermostats, in a wide sense, constitute a rich open field of research, see [1,10,12]. The interesting Wojtkowski [12], was the first to introduce thermostats in a general Riemann manifold (see [12, Eq. (1.7) with $W = 0$]).

2. Geodesic dynamics for general thermostats

First, let us introduce notations. When dealing with differentials of functions of two vector variables, x will be the first vector variable and y the second, while ∂ will be the symbol for differential, and the linear arguments will be enclosed in square brackets. The same symbol will be also used for the gradient vector (since we keep ∇ and "grad" for a later use in Section 4). The dot in $u \cdot v$ stands for the standard scalar product of vectors in $\mathbb{R}^n$.

Let us start with an open set $\Omega \subset \mathbb{R}^n \times \mathbb{R}^n$ and suppose we have two real-valued functions $L(x, y)$, the Lagrangian, and $b(x, y)$, a scalar constraint, of class C^2 on Ω. If I is an open interval in $\mathbb{R}$ and $q : I \to \mathbb{R}^n$ is a C^2 function, we follow d'Alembert–Lagrange principle (see the notion of perfect constraint in [9, p. 299]), and we say that q is a nonholonomic motion for the nonholonomic system defined by L and b if there exists $\lambda : I \to \mathbb{R}$, the "multiplier", such that for all $t \in I$

$$\begin{cases} (q(t), \dot{q}(t)) \in \Omega, \\ b(q(t), \dot{q}(t)) = 0, \\ \dfrac{d}{dt}\partial_y L(q(t), \dot{q}(t)) - \partial_x L(q(t), \dot{q}(t)) = \lambda(t)\partial_y b(q(t), \dot{q}(t)). \end{cases} \tag{2.1}$$

In particular, we are interested in the *natural Lagrangian functions* L

$$L(x, y) = K(x, y) - U(x), \quad K(x, y) = \tfrac{1}{2} y \cdot A(x) y, \tag{2.2}$$

where $x \in D$ open set of $\mathbb{R}^n$ (the configuration space) and $y \in \mathbb{R}^n$, the $n \times n$ matrix $A(x)$ is symmetric and positive definite at each point $x \in D$, the function K is called the *kinetic energy*, and U the *potential energy*. If one asks the mechanical system to keep a constant kinetic energy, then one has a *natural thermostatted system*, or briefly a (natural) thermostat. By means of a linear change of the time variable we can always normalize to $1/2$ the constant value of the kinetic energy. So the dynamics of a natural thermostat satisfies $q(t) \in D$ and the following system (we skip the dependence on t)

$$\begin{cases} \dot{q} \cdot A(q)\dot{q} = 1, \\ A(q)(\ddot{q} + \Gamma(q)[\dot{q}, \dot{q}]) + \partial U(q) = \lambda A(q)\dot{q}, \end{cases} \tag{2.3}$$

where $\partial U(x)$ is here the gradient vector (so $\partial U(x) \cdot y = \partial U(x)[y]$), while $\Gamma(x) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$, $(y, z) \mapsto \Gamma(x)[y, z]$, is the bilinear symmetric map (named after Christoffel in the classical books) given by

$$u \cdot A(x)\Gamma(x)[y, z] = \tfrac{1}{2}(\partial_x(u \cdot A(x)y)[z] + \partial_x(u \cdot A(x)z)[y] - \partial_x(z \cdot A(x)y)[u]). \tag{2.4}$$

Let us replace the constraint equation $K(q, \dot{q}) = 1/2$ by its time derivative

$$\dot{q} \cdot A(q)\ddot{q} + \partial_x K(q, \dot{q})[\dot{q}] = 0 \tag{2.5}$$

or equivalently

$$\dot{q} \cdot A(q)(\ddot{q} + \Gamma(q)[\dot{q}, \dot{q}]) = 0. \tag{2.6}$$

In this way system (2.3) implies a new system that can be put in Cauchy normal form with respect to $(\ddot{q}, \lambda)$

$$\begin{cases} \lambda = \dfrac{\partial U(q)[\dot{q}]}{\dot{q} \cdot A(q)\dot{q}}, \\ \ddot{q} = -\Gamma(q)[\dot{q}, \dot{q}] - A(q)^{-1}\partial U(q) + \dfrac{\partial U(q)[\dot{q}]}{\dot{q} \cdot A(q)\dot{q}}\dot{q}. \end{cases} \tag{2.7}$$

This system has the kinetic energy as first integral so, if we just consider the solutions with $\dot{q} \cdot A(q)\dot{q} = 1$ we then have precisely the set of all solutions of (2.3). Moreover, the last equation separates, namely does not depend on λ, so we can get rid of the multiplier λ. So we have arrived at the following Cauchy problems which give all motions of the natural system with thermostat

$$\begin{cases} (q(0), \dot{q}(0)) = (q_0, \dot{q}_0) \in \{(x, y) \in D \times \mathbb{R}^n : y \cdot A(x)y = 1\}, \\ \ddot{q} = -\Gamma(q)[\dot{q}, \dot{q}] - A(q)^{-1}\partial U(q) + \dfrac{\partial U(q)[\dot{q}]}{\dot{q} \cdot A(q)\dot{q}}\dot{q}. \end{cases} \tag{2.8}$$

This Cauchy problem has a unique solution being associated to a C^1 vector field (remind that A, U are of class C^2 so $\Gamma, \partial U$ are C^1) which is the unique solution to the slightly simpler system

$$\begin{cases} (q(0), \dot{q}(0)) = (q_0, \dot{q}_0) \in \{(x, y) \in D \times \mathbb{R}^n : y \cdot A(x)y = 1\}, \\ \quad \ddot{q} = -\Gamma(q)[\dot{q}, \dot{q}] - A(q)^{-1}\, \partial U(q) + (\partial U(q)[\dot{q}])\dot{q}. \end{cases} \tag{2.9}$$

So we have the following statement:

Proposition 2.1. *Let $D \subseteq \mathbb{R}^n$ be open and let the C^2 Lagrangian function $L : D \times \mathbb{R}^n \to \mathbb{R}$, $(x, y) \mapsto \frac{1}{2} y \cdot A(x)y - U(x)$ and the nonholonomic constraint $y \cdot A(x)y = 1$ define a natural thermostatted system. The Cauchy problems* (2.9) *give all thermostatted motions. More precisely, if q solves* (2.9), *then the pair (q, λ), with λ as in* (2.7), *is a solution of* (2.3), *vice-versa, if the pair (q, λ) is a solution of* (2.3), *then q satisfies the differential equation in* (2.9).

Incidentally, the thermostatted dynamics is not conservative, namely the *total energy* $K(q, \dot{q}) + U(q)$ is not a first integral unless U is trivial. Moreover, it is a reversible dynamics, that is $q(-t)$ is a motion as well as $q(t)$. A general theory on energy conservation and time-reversibility for nonlinear nonholonomic constraints is shown in [6].

Remark 2.2. For $n = 1$ the differential equation in (2.8) becomes $\ddot{q} = -\Gamma(q)[\dot{q}, \dot{q}]$, so we get the thermostatted dynamics by just ignoring the potential energy. The first integral $A(q)\dot{q}^2 = 1$ (where now $A(q) \in \mathbb{R}$) implies that q is strictly monotone and we always get dynamic convexity on an open interval $D \subseteq \mathbb{R}$. Example 2.4 will show that for $n > 1$ the problem of dynamic convexity is nontrivial.

Now, let us consider the solution to (2.9) and the change of time variable $\tau = T(t)$ given by

$$T(t) = \int_0^t e^{-U(q(s))}\, ds. \tag{2.10}$$

We denote by q the composed function $q \circ T^{-1}$ and by q$'$ its derivative at τ, while $\dot{\mathrm{q}}$ stands for the derivative of q calculated at $T^{-1}(\tau)$, so

$$\mathrm{q}' = \dot{\mathrm{q}} e^{U(\mathrm{q})}, \quad \mathrm{q}'' = \ddot{\mathrm{q}} e^{2U(\mathrm{q})} + \dot{\mathrm{q}} e^{2U(\mathrm{q})} \partial U(\mathrm{q})[\dot{\mathrm{q}}]. \tag{2.11}$$

By the last equation in (2.9) we then have

$$e^{-2U(\mathrm{q})} A(\mathrm{q})\mathrm{q}'' = -A(\mathrm{q})\Gamma(\mathrm{q})[\dot{\mathrm{q}}, \dot{\mathrm{q}}] - \partial U(\mathrm{q}) + 2A(\mathrm{q})\dot{\mathrm{q}} \partial U(\mathrm{q})[\dot{\mathrm{q}}]. \tag{2.12}$$

Let us introduce the following new matrix field on D

$$G(x) := e^{-2U(x)} A(x), \tag{2.13}$$

and Eq. (2.12) becomes

$$G(\mathrm{q})\mathrm{q}'' + G(\mathrm{q})\Gamma(\mathrm{q})[\mathrm{q}', \mathrm{q}'] - 2\partial U(\mathrm{q})[\mathrm{q}']G(\mathrm{q})\mathrm{q}' = -\partial U(\mathrm{q}). \tag{2.14}$$

We easily check that the equation for the geodesics of G (a Jacobi-like metric, see [11]), that is

$$\frac{d}{d\tau}\partial_y \mathscr{K}(\mathrm{q}, \mathrm{q}') - \partial_x \mathscr{K}(\mathrm{q}, \mathrm{q}') = 0, \quad \mathscr{K}(x, y) = \tfrac{1}{2} y \cdot G(x)y, \tag{2.15}$$

can be written as

$$G(\mathrm{q})\mathrm{q}'' + G(\mathrm{q})\Gamma(\mathrm{q})[\mathrm{q}', \mathrm{q}'] - 2\,\partial U(\mathrm{q})[\mathrm{q}']G(\mathrm{q})\mathrm{q}' = -(\mathrm{q}' \cdot G(\mathrm{q})\mathrm{q}')\partial U(\mathrm{q}), \tag{2.16}$$

(remind that Γ is always as in (2.4)) which differs from (2.14) for the right-hand side only. The last equation has $\mathrm{q}' \cdot G(\mathrm{q})\mathrm{q}'$ as first integral. If we just consider the solutions in the level 1 of this function we have solutions also to (2.14) since, in that case, the right-hand side of (2.16) is simply $-\partial U(\mathrm{q})$.

Proposition 2.3. *Let $D \subseteq \mathbb{R}^n$ be open and let the C^2 Lagrangian function $L : D \times \mathbb{R}^n \to \mathbb{R}$, $(x, y) \mapsto \frac{1}{2} y \cdot A(x)y - U(x)$ and the nonholonomic constraint $y \cdot A(x)y = 1$ define a natural thermostatted system. Then each solution q to* (2.9) (*each thermostatted motion*) *coincides with a geodesic* q *of* (2.13), *that is a solution of* (2.15), *on the level* 1 *of the first integral* $\mathrm{q}' \cdot G(\mathrm{q})\mathrm{q}'$, *up to the change of time variable* $\tau = T(t)$ *given by* (2.10).

Example 2.4. The Lagrangian function is $L(x, y) = \frac{1}{2}(y_1^2 + y_2^2) - \varepsilon x_1$, with $\varepsilon > 0$, and the nonholonomic constraint is $y_1^2 + y_2^2 = 1$. This thermostatted system is physically interesting since it is part of a model for electrical conduction called *the Lorentz gas* (which also includes elastic collisions with scatterers which are not of our concern), see [4,10]. System (2.9) becomes

$$\begin{cases} (q(0), \dot{q}(0)) = (q_0, \dot{q}_0) \in \{(x, y) \in \mathbb{R}^2 \times \mathbb{R}^2\colon\ y \cdot y = 1\}, \\ \qquad \ddot{q}_1 = -\varepsilon + \varepsilon \dot{q}_1^2, \quad \ddot{q}_2 = \varepsilon \dot{q}_1 \dot{q}_2. \end{cases} \tag{2.17}$$

Equivalently

$$\begin{cases} (q(0), \dot{q}(0)) = (q_0, \dot{q}_0) \in \{(x, y) \in \mathbb{R}^2 \times \mathbb{R}^2\colon\ y \cdot y = 1\}, \\ \qquad \ddot{q}_1 = \dfrac{\varepsilon}{2}(-1 + \dot{q}_1^2 - \dot{q}_2^2), \quad \ddot{q}_2 = \varepsilon \dot{q}_1 \dot{q}_2. \end{cases} \tag{2.18}$$

By introducing the complex valued function $z(t) = \varepsilon(q_1(t) + iq_2(t))$, the previous system becomes

$$\begin{cases} (z(0), \dot{z}(0)) = (z_0, \dot{z}_0) \in \mathbb{C} \times \mathbb{S}^1, \\ \qquad \ddot{z} = \frac{1}{2}(-1 + \dot{z}^2). \end{cases} \tag{2.19}$$

Remark that, by defining $u = \dot{z}$, the last equation is $\dot{u} = (-1 + u^2)/2$ which has the unit circle $\mathbb{S}^1$ as invariant set. The solution of (2.19) can be written by means of the principal logarithmic function

$$z(t) = z_0 + t + \log \frac{4}{(1 + e^t(1 - \dot{z}_0) + \dot{z}_0)^2}. \tag{2.20}$$

This shows that the imaginary part of $z(t) - z_0$ belongs to $]-\pi, \pi[$. Returning back to q, the conclusion is that from the initial point (x_1, x_2) we can only reach points in the strip $\mathbb{R}\times]x_2 - \pi/\varepsilon, x_2 + \pi/\varepsilon[$ (Fig. 1).

Another way to look at this result is by considering the geodesics of (2.13) which in the actual case becomes

$$G(x_1, x_2) \coloneqq e^{-2\varepsilon x_1} I, \tag{2.21}$$

where I is the identity 2×2 matrix. Consider the function

$$f : \mathbb{R}^2 \to \mathbb{R}^2, \quad (x_1, x_2) \mapsto e^{-\varepsilon x_1}(\cos(-\varepsilon x_2), \sin(-\varepsilon x_2)) \tag{2.22}$$

then we can check that $\varepsilon^2 G(x_1, x_2) = f'(x_1, x_2)^T f'(x_1, x_2)$ the product of the transpose Jacobian matrix and the Jacobian matrix of f. So for any geodesic $\mathrm{q}(\tau)$ (see (2.15)) we have that $f(\mathrm{q}(\tau))$ is an affine function. Equivalently, the complex valued map $e^{-z(\tau)}$ is an affine function of the real variable τ if $z(\tau) = \varepsilon q(\tau)$, and we reach the aforementioned conclusions at once.

So we have just seen that the thermostatted system is not dynamically convex. On the contrary, the dynamical system defined by $L(x_1, x_2, y_1, y_2) = \frac{1}{2}(y_1^2 + y_2^2)$, without nonholonomic constraints, which has $y_1^2 + y_2^2$ as first integral, is dynamically convex

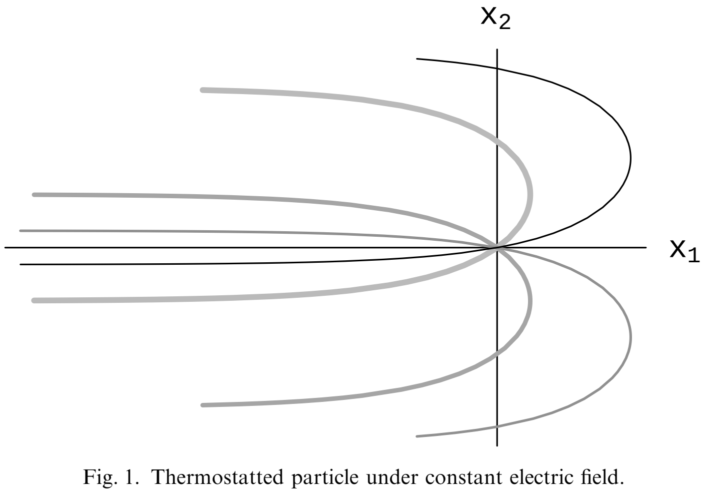

Fig. 1. Thermostatted particle under constant electric field.

and this is of course true even if we just consider the solutions with $y_1^2 + y_2^2 = 1$ which holds for the thermostatted system too.

3. Dynamic convexity on Euclidean n-space

We are going to see a sufficient condition for the dynamic convexity of a thermostat which involves the usual operator norm $||A(x)^{-1}|| = \sup\{|A(x)^{-1} u|\colon |u| = 1\}$.

Proposition 3.1. *Let the C^2 Lagrangian function $L : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, $(x, y) \mapsto \frac{1}{2} y \cdot A(x)y - U(x)$, and the nonholonomic constraint $y \cdot A(x)y = 1$ define a natural thermostatted system, moreover let*

$$\sup\{e^{2U(x)} ||A(x)^{-1}||\colon x \in \mathbb{R}^n\} < +\infty. \tag{3.1}$$

Then, for any choice of two points $\hat{x}, \tilde{x} \in \mathbb{R}^n$, there exists a thermostatted motion $q : I \to \mathbb{R}^n$ which joins them, that is such that $\hat{x}, \tilde{x} \in q(I)$.

Proof. Let us denote by a the supremum in (3.1). Consider a geodesic of the metric (2.13), namely a solution $J \to \mathbb{R}^n$, $\tau \mapsto \mathrm{q}(\tau)$ of (2.15), where J is the maximal interval of existence. By the first integral of energy $\mathscr{K}$, there exists $E > 0$ such that for every $\tau \in J$

$$\frac{2E}{|\mathrm{q}'(\tau)|^2} = \frac{\mathrm{q}'(\tau)}{|\mathrm{q}'(\tau)|} \cdot G(\mathrm{q}(\tau)) \frac{\mathrm{q}'(\tau)}{|\mathrm{q}'(\tau)|} \geqslant \mu(\mathrm{q}(\tau)) \tag{3.2}$$

where $\mu(x)$ is smallest eigenvalue of $G(x)$. So

$$|\mathrm{q}'(\tau)|^2 \leqslant \frac{2E}{\mu(\mathrm{q}(\tau))} \leqslant 2E||G(\mathrm{q}(\tau))^{-1}|| = 2Ee^{2U(\mathrm{q}(\tau))}||A(\mathrm{q}(\tau))^{-1}|| \leqslant 2Ea. \tag{3.3}$$

Standard arguments in ordinary differential equations then permit us to reach the conclusion that the maximal interval of existence J is actually the whole $\mathbb{R}$. Since all geodesics are defined on the whole real line, then we can invoke Hopf–Rinow's theorem (see for instance [7]) to state the existence of one of them which joins $\hat{x}, \tilde{x} \in \mathbb{R}^n$. Now an affine change of time gives a geodesic $\mathrm{q}(\tau)$ which keeps joining $\hat{x}, \tilde{x}$, is defined at $\tau = 0$, and is such that $\mathrm{q}' \cdot G(\mathrm{q})\mathrm{q}' = 1$. As we saw in the lines after (2.16), this is also a solution to (2.14). The change of variable whose inverse is

$$T^{-1}(\tau) = \int_0^\tau e^{U(\mathrm{q}(\xi))}\, d\xi, \tag{3.4}$$

gives thermostatted motion $q : I \to \mathbb{R}^n$, $t \mapsto \mathrm{q}(T(t))$ which joins $\hat{x}, \tilde{x} \in \mathbb{R}^n$, that is which satisfies $\hat{x}, \tilde{x} \in q(I)$. $\square$

In the previous proof, we have showed that the geodesics of G are defined on the whole $\mathbb{R}$. Of course, this does not mean that the thermostatted motions are globally defined too (as one may see on examples with $n = 1$).

Example 3.2. By Proposition 3.1, the following modification of the Example 2.4 yields dynamically convex thermostats:

$$L(x,y) = K(x,y) - \varepsilon x_1 - f(x), \quad K(x,y) = \tfrac{1}{2} e^{2\varepsilon x_1}(y_1^2 + y_2^2), \quad x, y \in \mathbb{R}^2, \tag{3.5}$$

where $f : \mathbb{R}^2 \to \mathbb{R}$, is an arbitrary bounded from above smooth function, and the nonholonomic constraint is $e^{2\varepsilon x_1}(y_1^2 + y_2^2) = 1$.

Let us see that the unconstrained dynamical system with the same kinetic energy and no potential is not dynamically convex. The motion is ruled by

$$\frac{d}{dt}\partial_y K(q, \dot{q}) - \partial_x K(q, \dot{q}) = 0, \tag{3.6}$$

namely

$$e^{2\varepsilon q_1}(\ddot{q}_1 + \varepsilon \dot{q}_1^2 - \varepsilon \dot{q}_2^2) = 0, \quad e^{2\varepsilon q_1}(\ddot{q}_2 + 2\varepsilon \dot{q}_1 \dot{q}_2) = 0. \tag{3.7}$$

By introducing the complex valued function $z(t) = \varepsilon(q_1(t) + iq_2(t))$, the previous system becomes

$$\ddot{z} + \dot{z}^2 = 0. \tag{3.8}$$

The solution with $z(0) = z_0$, and $\dot{z}(0) = \dot{z}_0$, is

$$z(t) = z_0 + \log(1 + t\dot{z}_0). \tag{3.9}$$

This shows that the imaginary part of $z(t) - z_0$ belongs to $]-\pi, \pi[$. Returning back to q, the conclusion is that from the initial point (x_1, x_2) we can only reach points in the strip $\mathbb{R}\times]x_2 - \pi/\varepsilon, x_2 + \pi/\varepsilon[$.

We are going to see another sufficient condition of dynamic convexity. This condition involves an auxiliary function $k : D \to \mathbb{R}$ which is *proper*, namely it is a continuous function, and the inverse images of compact sets are compact. In the particular case of $D = \mathbb{R}^n$ this last condition is equivalent to coercitivity, that is $k(x) \to +\infty$ as $x \to \infty$. In the following statement, the symbol $\partial k(x)$ is used for the gradient vector.

Theorem 3.3. *Let $D \subseteq \mathbb{R}^n$ be open and connected, and let the C^2 Lagrangian function $L : D \times \mathbb{R}^n \to \mathbb{R}$, $(x,y) \mapsto \frac{1}{2} y \cdot A(x)y - U(x)$, and the nonholonomic constraint $y \cdot A(x)y = 1$ define a natural thermostatted system. If there exists a proper function $k : D \to \mathbb{R}$, of class C^1 and such that*

$$\sup\{e^{2U(x)}\partial k(x) \cdot A(x)^{-1}\partial k(x) \colon x \in D\} < +\infty, \tag{3.10}$$

then, for any choice of two points $\hat{x}, \tilde{x} \in D$, *there exists a thermostatted motion* $q : I \to \mathbb{R}^n$ *which joins them, that is such that* $\hat{x}, \tilde{x} \in q(I)$.

Proof. Let us denote by a the supremum in (3.10) which is a positive number. Consider a solution $[0, b[\to \mathbb{R}^n$, $\tau \mapsto \mathrm{q}(\tau)$ of (2.15), with $0 < b < +\infty$. By the first integral of energy $\mathscr{K}$, there exists $E > 0$ such that $2E = \mathrm{q}'(\tau) \cdot G(\mathrm{q}(\tau))\mathrm{q}'(\tau)$ for all $\tau \in [0, b[$. We have

$$\begin{aligned} \left|\frac{d}{d\tau} k(\mathrm{q}(\tau))\right| &= |\partial k(\mathrm{q}(\tau))[\mathrm{q}'(\tau)]| = |\mathrm{q}'(\tau) \cdot G(\mathrm{q}(\tau))(G(\mathrm{q}(\tau))^{-1}\partial k(\mathrm{q}(\tau)))| \\ &\leqslant \sqrt{\mathrm{q}' \cdot G(\mathrm{q}(\tau))\mathrm{q}'}\sqrt{(G^{-1}\partial k) \cdot G(\mathrm{q}(\tau))(G^{-1}\partial k)} = \sqrt{2E}\sqrt{a}, \end{aligned} \tag{3.11}$$

where we have used the Schwarz inequality applied to the scalar product defined by G (that is $u \cdot Gv$). Therefore, for all $\tau \in [0, b[$

$$|k(\mathrm{q}(\tau))| \leqslant |k(\mathrm{q}(0))| + b\sqrt{2E}\sqrt{a} =: c. \tag{3.12}$$

Now, since the function k is proper, then the inverse image of the compact interval $[-c, c]$ is a compact subset of D which contains the geodesic. By this fact, and by the integral of energy, we have that $(\mathrm{q}(\tau), \mathrm{q}'(\tau))$ is trapped into a compact subset of $D \times \mathbb{R}^n$. Indeed, let m be the minimum value of the smallest eigenvalue $\mu(x)$ of $G(x)$ on the compact set $k^{-1}([-c, c])$, then

$$\frac{2E}{|\mathrm{q}'(\tau)|^2} = \frac{\mathrm{q}'(\tau)}{|\mathrm{q}'(\tau)|} \cdot G(\mathrm{q}(\tau)) \frac{\mathrm{q}'(\tau)}{|\mathrm{q}'(\tau)|} \geqslant \mu(\mathrm{q}(\tau)) \geqslant m > 0 \tag{3.13}$$

and $|\mathrm{q}'(\tau)| \leqslant \sqrt{2E/m}$. Therefore the geodesic is extendible in the future by standard arguments of ODEs. This shows that all maximal geodesics are defined on the whole $\mathbb{R}$ and the result follows from Hopf–Rinow's theorem as in the proof of Proposition 3.1. $\square$

As a noteworthy example let us mention the proper function

$$k : \mathbb{R}^n \to \mathbb{R}, \quad x \mapsto \tfrac{1}{2}\log(1 + |x|^2). \tag{3.14}$$

By using k as an auxiliary function (on the whole $\mathbb{R}^n$), we get the following particular case of condition (3.10)

$$\sup\left\{ e^{2U(x)} \frac{x \cdot A(x)^{-1}x}{(1 + |x|^2)^2} \colon\ x \in \mathbb{R}^n \right\} < +\infty. \tag{3.15}$$

Under condition (3.1), this is certainly true. So we have found Proposition 3.1 as a corollary of Theorem 3.3. However, condition (3.15) provides a wide class of examples, among which the following ones.

Example 3.4. By condition (3.15), the following Lagrangian functions give dynamically convex thermostats

$$L(x,y) = \tfrac{1}{2}|y|^2 - \tfrac{1}{2}\log(1+|x|^2) - f(x), \quad x, y \in \mathbb{R}^n, \tag{3.16}$$

where f is an arbitrary bounded from above smooth function.

4. Thermostatted dynamics on Riemannian manifolds

All we have said in the preceding section can be generalized to Riemannian manifolds. Let M be a smooth n-dimensional connected manifold with a Riemannian metric $\langle\, , \rangle$, and let ∇ be the Levi–Civita affine connection defined by the metric (see for instance [7]). The kinetic energy is the function $K : TM \to \mathbb{R},\ v \mapsto \langle v, v\rangle/2$, on the tangent bundle. We assume a smooth potential energy function $U : M \to \mathbb{R}$ is given too. Following [7] we denote by grad U the vector field defined by $\langle \operatorname{grad} U(x), v\rangle = \partial U(x)[v]$ for any point $x \in M$ and $v \in T_x M$, the tangent space at x. So, if the positive symmetric matrix field A realizes the scalar product in a local coordinate system, we then have the following formula which gives the i-component of the grad in terms of the partial derivatives $\partial_j U$ and of the components of A^{-1}

$$(\text{grad } U)_i = \sum_j A^{-1}_{ij} \partial_j U. \tag{4.1}$$

If $\gamma : t \mapsto \gamma(t)$ is a smooth curve in M, the symbol $\nabla\dot\gamma(t)$ denotes the covariant derivative of the tangent vector $\dot\gamma(t)$. For the thermostatted dynamics we introduce the equations

$$\begin{cases} \langle \dot\gamma(0), \dot\gamma(0)\rangle = 1, \\ \nabla\dot\gamma(t) + \text{grad } U(\gamma(t)) = \partial U(\gamma(t))[\dot\gamma(t)]\dot\gamma(t), \end{cases} \tag{4.2}$$

which give $\langle \dot\gamma(t), \dot\gamma(t)\rangle = 1$ along the solutions. In a local coordinate system the thermostatted dynamics (4.3) reduces to (2.9).

Let $\sigma : [0, b[\to M,\ \tau \mapsto \sigma(\tau)$, be a geodesic of the new metric $e^{-2U}\langle\, , \rangle$, namely a solution of

$$\tilde\nabla \sigma'(\tau) = 0, \tag{4.3}$$

where $\tilde\nabla$ is the Levi–Civita connection of the new metric and we have denoted by $\sigma'(\tau)$ the tangent vector. Then, whenever the first integral $e^{-2U(\sigma(\tau))}\langle \sigma'(\tau), \sigma'(\tau)\rangle = 1$, we have a reparametrization of a thermostatted motion $t \mapsto \gamma(t)$ by the change of time variable $\tau = T(t)$ given by

$$T(t) = \int_0^t e^{-U(\gamma(s))}\, ds. \tag{4.4}$$

The proof was already done in Section 2 with minor changes to consider the equations there as the actual ones in a local chart.

Our previous result, Theorem 3.3, is easily generalized to the present situation.

Theorem 4.1. *Let M be a smooth connected finite-dimensional manifold with a Riemannian metric $\langle\, ,\, \rangle$, and let $U : M \to \mathbb{R}$ be a smooth function on M. If there exists a smooth proper function $k : M \to \mathbb{R}$ such that*

$$\sup\{e^{2U(x)}\langle \operatorname{grad} k(x), \operatorname{grad} k(x)\rangle : \; x \in M\} < +\infty, \tag{4.5}$$

then, for any choice of two points $\hat{x}, \tilde{x} \in M$, there exists a thermostatted motion $\gamma : I \to M$ which joins them, that is a solution to (4.2) *such that $\hat{x}, \tilde{x} \in \gamma(I)$.*

Proof. The proof is the same (mutatis mutandis) as the one of Theorem 3.3 till formula (3.12) which holds also in the actual general case. Then we use the properness of k to say the inverse image of the compact interval $[-c, c]$ is a compact subset C of M which contains the geodesic. Since M is paracompact, C is the finite union of compact sets, $C = U_j C_j$, each one of them being contained in the domain of a local coordinate system. So we may argue as in the proof of Theorem 3.3 to get a compact subset K_j of TM, whose projection on M is C_j, and finally $K = U_j K_j$ a compact subset of TM such that $\sigma'([0, b[) \subseteq K$. The conclusion follows as in the proof of Theorem 3.3. $\square$

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